

Center Reflections

A monthly publication highlighting activities at the W.M. Keck Foundation Center for Molecular Structure

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American Crystallographic Association National Meeting to Be Held in Los Angeles in 2001

The American Crystallographic Association (ACA) represents the community of North American crystallographers. Members of the ACA may also be elected to the U.S. National Committee for Crystallography, which represents North American crystallographers in the International Union of Crystallography (IUCr). The aim of the ACA is to promote the advancement of the science of crystallography in North America.

Each year, the ACA holds a national meeting, which is chaired by local crystallographers. In 2001, the ACA meeting will be held at the Bonaventure Hotel in downtown Los Angeles. The local co-chairs are Dr. Dan Anderson of the DOE Structural Biology Laboratory at UCLA, and Professor Katherine Kantardjieff of CSU Fullerton and Director of CMoLS. Program Chair for the meeting is Dr. Duncan McRee of The Scripps Research Institute. The preliminary program includes the Transaction Symposium on High Throughput Crystallography, as well as sessions on Difficult/Problem Structures and Hot New Methods. In addition, the Service Crystallography Special

Interest Group is sponsoring a symposium on Education in Crystallography.

The ACA recognizes contributions to the field by a number of memorial awards. Some of these are awarded annually, such as the Elizabeth Wood Award, given for demonstrated excellence in science writing, not necessarily by a scientist. In 2001, this award will be presented to K.C. Cole, chief science writer for the Los Angeles Times. Several awards, which are presented every three years, will be presented in Los Angeles: 1) the Warren Diffraction Physics Award, which recognizes an important recent contribution to the physics of solids or liquids using X-ray, neutron, or electron diffraction techniques; 2) the A.L. Patterson Award, which recognizes and encourages outstanding research in the structure of matter by diffraction methods, including significant contributions to the methodology of structure determination and/or innovative application of diffraction methods and/or elucidation of biological, chemical, geological or physical phenomena using new structural information; and 3) the Fankuchen Memorial Award, which recognizes contributions to crystallographic research by one who is known to be an effective teacher of crystallography. We are pleased to announce that Katherine Kantardjieff has been nomi-

nated for the Fankuchen Memorial Award for her pioneering efforts to develop crystallography research and curriculum, as well as remote access to instrumentation in a predominantly undergraduate institution.

After the new year, Katherine will be seeking students to assist with the meeting operations as guides, audio-visual coordinators, etc. Students will be paid hourly rates and will be given hotel accommodations. If any of you at CSUs in the LA Basin know of students who would be interested in this opportunity, please have them contact Katherine Kantardjieff.

Remote Access to the National Synchrotron Light Source



The U.S. Department of Energy's Brookhaven National Laboratory creates and operates major facilities available to university, industrial and government personnel for basic and applied research in physical, biomedical and environmental sciences, as well as in selected energy technologies. BNL is an NIH-sponsored resource for macromolecular crystallography, which includes remote access to beamlines. This has affectionately been dubbed "Fedex crystallography" by the structural biologists among us.

In response to the growing need for frequent synchrotron time by the protein crystallographic community in the era of structural genomics, a relatively inexpensive and effi-

cient means of beamline operation has been developed, called "Fedex data collection", where users send their crystals to the synchrotron beamline and local beamline personnel collect data for the users while interacting via the wonders of modern technology. This is similar to the remote access capabilities at CMoLS available to faculty and students throughout the CSU. "Fedex data collection" is now operational at beamline X12C at the NSLS, where an attractive suite of tools for remote monitoring and partial control of beamline operations is available. Ideal cases for this mode of operation are those involving multiple anomalous dispersion or MAD data collection, but it is also possible to collect native, derivative, or high-resolution data. In some circumstances, crystal screening can be done.

Dr. Robert M. Sweet, who heads this project at BNL, has agreed to provide CMoLS the opportunity to take advantage of Fedex data collection. What you will need to do is contact Katherine Kantardjieff with your needs. She will then schedule beamtime with BNL. Katherine and CMoLS staff can assist you with preparing samples and sending BNL a dry dewar with your crystals already cryo-cooled, so that it will arrive on a weekday, 1 to 3 days before the scheduled data collection. Only certain types and heights of sample pins are suitable for the beamline. CMoLS will familiarize you with the beamline, particularly if you intend to participate significantly in remote operation of the beamline, and CMoLS will arrange for remote logins and passwords. BNL staff will add liquid N₂ to your dewar immediately when they receive it, mount the crystals, set up the data collection, and collect data.

An initial processing will normally be done locally. After this, you or CMoLS staff can ftp files during data collection to begin structure solution. Processing is typically done by a version of DENZO that allows

processing of data from the Brandeis detectors. Alternatively, other programs capable of handling images from these detectors may be used. If you want to do a MAD (or SAD) experiment, the program CHOOCH can be run locally to estimate f and f' followed by SOLVE. CMolS can also prepare to estimate these values whatever way you choose. Data will be archived on DAT at BNL and returned to you or CMolS.

Bob has agreed to allow CMolS to use this remote access to the beamline on occasion for training purposes. We are planning to include a session on Fedex data collection at our "Crystallography for Chemists" workshop in January, 2001. If you would be interested in participating in such a session, please let us know.

The TB Structural Genomics Consortium

The TB Structural Genomics Consortium proposes to demonstrate the power of structural genomics by using it to address a significant problem in human health, the pathogenicity of *Mycobacterium tuberculosis*. The Consortium will determine and analyze the structures of over 400 functionally important proteins from *M. tuberculosis*. The database of structural and functional information that it constructs will form a basis for understanding *M. tuberculosis* pathogenesis and will enable structure-based design of novel drugs. The structures will include about 40 novel folds and 200 new structural families, providing a foundation for structure prediction of related proteins.

To accomplish this, The Consortium has developed an approach that will deliver structures and analyses of high value in a cost-effective manner. The Consortium will target functionally important proteins through the use of genetic screens and genome-scale functional assignments. The Consortium

will use its green fluorescent protein-based screening system to optimize proteins for expression, solubility and methionine content. Crystallization will be carried out by a low-cost system that combines automation of a stochastic screening protocol with image analysis of droplets. The Consortium will emphasize selenomethionine MAD X-ray data collection on characterized crystals at synchrotron facilities, with concurrent structure solution using automated software. Synchrotron time sufficient for collection of 300 MAD structures per year has been secured for this program. Structural data will be systematically analyzed for fold assignment, similarity to other proteins, and local motifs. Analysis of structures determined will use new function prediction methods that will guide biochemical tests of function.

Members will implement a consortium approach to structural genomics that allows a worldwide effort to be focused on a defined set of targets. The TB Structural Genomics Consortium consists of 24 laboratories from 13 institutions in 6 countries.* Consortium laboratories are collectively responsible for 3.3% of all protein structures in the Protein Data Bank and have extensive records of methods development. Consortium members have carried out a pilot project on the structural genomics of a hyperthermophile that has identified bottlenecks and resulted in development of methodologies for high-throughput structure determination and analysis. The Consortium will have centralized facilities that will carry out an increasing fraction of routine tasks such as protein production, crystallization and X-ray data collection. The structural and functional information obtained in this project is to be placed in the public domain by timely deposition in publicly available databases.

*The TB Structural Genomics Consortium: Thomas Alber, James Berger, University of

California, Berkeley; Edward N. Baker, University of Auckland; Joel Berendzen, Min Park, Tom Terwilliger, Geoffrey Waldo, Los Alamos National Laboratory; James Bowie, David Eisenberg, Juli Feigon, Jeanne Perry, Todd Yeates, UCLA; Axel Brunger, Paul Adams, Lawrence Berkeley National Laboratory; William Jacobs, Albert Einstein College of Medicine; Bernhard Rupp, Lawrence Livermore National Laboratory; James Sacchettini, Texas A&M University; Se Won Suh, Seoul National University; Manfred Weiss, Institute of Molecular Biology, Jena; Matthias Wilmans, Paul Tucker, Emke Pohl, Victor Lamzin, EMBL-Hamburg; William Wood, University of Colorado, Boulder; Shigeyuki Yokoyama, RIKEN, Janet Thornton, University College, London; Guy Dodson, University of York; Charles Carter, University of North Carolina, Chapel Hill; Katherine Kantardjieff, California State University, Fullerton.

Websites of Interest

American Crystallographic Association
<http://nexus.hwi.buffalo.edu/aca/index.html>

International Union of Crystallography
<http://www.iucr.org/>

Xtal Nexus Internet Crystallography Software Library and Virtual WWW
<http://www.unige.ch/crystal/stxnews/nexus/index.htm>

CCP14: Collaborative Computational Project Number 14 for Single Crystal and Powder Diffraction (freely available crystallographic software for academia) <http://www.ccp14.ac.uk>

Upcoming Events

September 26, 2000: **San Jose State University** "X-ray Diffraction Studies in a Predominantly Undergraduate Institution". Seminar given by Prof. Katherine Kantardjieff to the Department of Chemistry and Biochemistry.

August 20 - 24, 2000: **American Chemical Society National Meeting**, Washington, DC.

October 25-28, 2000: **American Chemical Society Western Regional Meeting**, San Francisco, CA.
<http://www.mcs.csu Hayward.edu/~wwwchem/>

December 14 - 19, 2000: **Pacificchem 2000**, Honolulu, Hawaii.
<http://www.acs.org/meetings/pacific2000/>

January 2000: **Crystallography for Chemists Workshop**, CSU Fullerton.

January 2000: **CSUPERB Symposium**, Cal Poly Pomona.

July 21-26, 2001: **American Crystallographic Association National Meeting**, Los Angeles, CA.
<http://www.hwi.buffalo.edu/ACA/ACA-Annual/LosAngeles/LosAngeles.html>

March 2000: **West Coast Protein Crystallography Workshop**, Asilomar, CA.

April 1 - 5, 2001: **American Chemical Society National Meeting**, San Diego, CA.

April 18-22, 2001: **4th European Protein Symposium**, Paris, France.
<http://www.faseb.org/meetings/ep01/>

August 26 - 30, 2001: **American Chemical Society National Meeting**, Chicago, IL.

August 6-15, 2002: **International Union of Crystallography Meeting**, Jerusalem, Israel.
<http://www.iucr.org/>

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Staff Scientist: See job posting on website.